

Department of Chemistry, Texas A&M University-Kingsville

Chemistry Seminar Series

Wednesday, April 23, 2025, Peacock Auditorium (BES-100), 3:00 – 4:00 PM

ZOOM LINK: [https://tamuk-edu.zoom.us/j/6769157893?pwd=Y29YS-](https://tamuk-edu.zoom.us/j/6769157893?pwd=Y29YS-TBxeEJVOU1JVkh2MHlXZG5yUT09)

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What Makes a Protein Neurotoxic? Deep Learning Suggests a Strong Answer in Sequence Alone



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Predicting neurotoxicity from protein sequences remains a fundamental challenge due to the high structural variability and functional complexity of venom peptides across diverse animal lineages, including cone snails, scorpions, spiders, and snakes. This leads to a central question: can deep learning models extract meaningful sequence-level features that define neurotoxic activity? We developed a neural network achieving 96% classification accuracy, with consistently high performance across training and test datasets. To evaluate its sensitivity, we introduced sequence warping—strategic perturbations at conserved residues—to simulate natural mutations. Despite minimal changes to global sequence identity, predicted neurotoxicity sharply declined, and

structural modeling revealed disrupted binding-site architectures. These results suggest that deep learning can uncover latent, functionally critical signatures of neurotoxicity embedded within primary amino acid sequences. This approach offers new opportunities for venom-based drug discovery, evolutionary studies, and the design of bioactive peptides with tunable toxicity.

Short Biography:

Anas Bedraoui is a PhD student at the Faculty of Medical Sciences, UM6P, Morocco, and a Visiting Scholar in the Human Genetics Department at UTRGV. His work focuses on developing computational tools to analyze real-world biomedical data, blending artificial intelligence, toxinology, and high-throughput biology, particularly proteomics and metabolomics, to address complex challenges in health and science. He is currently a member of the Early Career Advisory Group at eLife at Cambridge, UK. Anas has published several articles and books and has received multiple awards for his contributions to research, including a prestigious innovation award for developing a brain-controlled bionic arm.